ASCI Three-Dimensional Hydrodynamic Instability and Turbulence Modeling

Mission

The ASCI fluid turbulence team studies turbulence processes in strongly-compressible three-dimensional hydrodynamic flows and develops subgrid-scale parameterizations of turbulence effects for large-eddy numerical simulations.

In many hydrodynamics applications, the relevant length scales range over several orders of magnitude, so that finite-difference direct numerical simulations (DNS) are computationally not feasible for the driving parameters of interest. To simulate the dynamically important range of scales, we will perform large-eddy simulations (LES) instead. Using LES, the dynamical effects of the unresolved scales are modeled by a subgrid-scale parameterization, and the resolved scales are calculated explicitly. These parameterizations allow the use of fewer grid points than would be necessary for a DNS. A major thrust of the ASCI applications programs is a shift from two-dimensional to three-dimensional physics computations. Turbulence in two and three dimensions is profoundly different, and the subgrid scale parameterizations developed for 2-D flow are generally insufficient for modeling 3-D flow. Thus, a principal research topic in this project is to develop subgrid-scale parameterizations from 3-D hydrodynamic theory and experiments and to validate them against fully resolved DNS and available experimental data.

Numerical Approach and Programming Model

We are using several numerical simulation codes, predominately one based on the piecewise parabolic method (PPM), which is a higher-order accurate Godunov method developed by Colella and Woodward. The Godunov approach is typical of standard numerical techniques in regions where the solution is smooth. However, in regions with discontinuities, such as strong shocks, the Godunov method approximates the solution well by analytically solving an associated Riemann problem. This is an idealized problem describing the evolution of a simple jump into shocks and/or rarefactions, with a contact discontinuity in between. Monotonicity constraints ensure that these discontinuities remain sharp and accurate as they traverse the computational grid. The higher-order spatial interpolation in the PPM allows steeper representation of discontinuities, thus allowing a more accurate solution to a wider class of problems. For some of our simulations, molecular dissipation processes are explicitly modeled, in which case the simulations are of the Navier-Stokes equations rather than the Euler equations. Parallelization across computational nodes is implemented by domain decomposition with message-passing. The subdomains are three-dimensional and contain extra border cells to allow intermediate computation, thereby reducing the required interprocessor communication. Variables are ordered in memory to effect optimal usage of cache. To date, we have run calculations on the IBM-SP, the INTEL Tflops machine, the DEC Alpha machine, and the T3D.

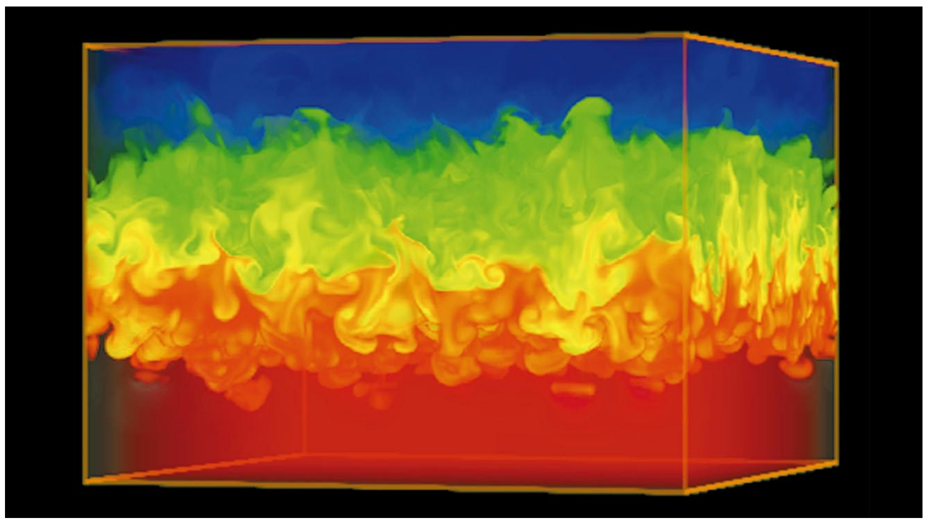

Figure 1. Mixing of the heavier fluid, which is initially on top, with the fluid on the bottom is known as the Rayleigh-Taylor instability.

Rayleigh-Taylor Instability

As an example of our research, we use the PPM code to simulate the Rayleigh-Taylor instability and turbulent mixing on a unit cube spanned by a grid containing 512 points in each of the three directions. This case was run on the ASCI Blue Pacific ID System using 128 nodes. The initial equilibrium state consists of a $\gamma = 5/3$ gas, in which the subvolumes above and below the midplane are stably stratified equilibria. The internal energies are piecewise constant, while the density and pressure decrease exponentially with height, but have different scale heights above

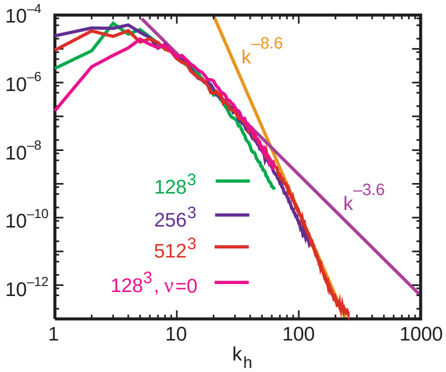

Figure 2. The spectra of vertical velocity at the midplane with respect to horizontal wave number, as a function of grid resolution, for the Rayleigh-Taylor problem.

and below the midplane. The density jumps by a factor of 2 from below to above the midplane, corresponding to an Atwood number of 1/3, while the pressure is continuous. The sound speed corresponding to the equilibrium state below the midplane is 1.0. The simulation includes molecular dissipation with a Prandtl number of 1.0. The boundaries are periodic in the horizontal directions and impenetrable in the vertical direction. A random spectrum of low-level velocity perturbations away from the equilibrium state is initially imposed. After the initial linear mixing phase, bubbles (rising from below) and spikes (falling from above) begin to form. Afterward, the horizontal fluctuation scales grow in size and the physical system evolves toward a stably stratified equilibrium. Figure 1 shows the temperature field at time $t = 4.0$. Figure 2 shows the spectra of vertical velocity (in terms of squared amplitude per mode) at the midplane as a function of horizontal wave number for various grid resolutions. The $512 \times 512 \times 512$ case appears to be converged (with respect to grid resolution), with the middle portion of the curve representing a possible inertial range.

Richtmyer-Meshkov Instability

A second example of our work involves simulating the Richtmyer-Meshkov instability, which is the impulsive-acceleration limit of the Rayleigh-Taylor instability. This instability occurs, for example, when a shock passes through an interface of two fluids of differing density. We consider an elongated domain having dimensions $0.5 \times 0.5 \times 1.37$, spanned by a $192 \times 192 \times 448$ mesh. A gas having a 2-fold density contrast across a single-mode perturbed planar interface impinges on a higher-density, higher-pressure gas to initiate a highly supersonic (Mach 6) shock on the low-density side of the contact discontinuity. We advect a passive scalar field that measures the degree of mixing of the low- and high-density fluids. Figure 3(a) shows the passive scalar in the aftermath of the interaction of the shock with the contact discontinuity. The development of fine-scale, non-chaotic features is evident. Figures 3(b) and 3(c) depict the result of passing an additional Mach 6 shock through the interface from the same and opposite sides, respectively. There is a distinct change in character, as much of the fine-scale structure is smeared out. Figure 4 shows the width of the mixing layer (measured by the departure of the passive scalar from its initial values) as a function of time. For the second shock phase (rightmost curve), the diamonds indicate the case where the second shock is in the same direction as the first, and the crosses indicate the case where the second shock is coming from the opposite side. The solid curves represent logarithmic fits, and the dashed curves are power law fits. The for-

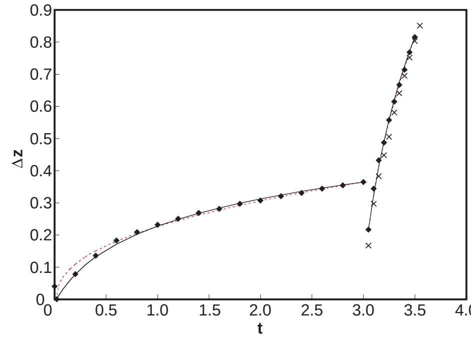

Figure 4. The width of the mixing layer as a function of time, for the Richtmyer-Meshkov instability.

ward and reverse shock cases differ by only a slight delay.

Evaluation of High-Performance Computing Platforms

This project has an important secondary goal, that of exploring the limits of ASCI high-performance computing platforms for three-dimensional hydrodynamics applications. This would include scalable, distributed memory massively parallel processors as well as shared memory processor clusters. Our high demands on data storage, visualization, and archival storage will test the robustness of the problem-solving environment as well.

We are collaborating with Paul Woodward and David Porter of the University of Minnesota, with Andrzej Domaradzki of the University of Southern California, and with Steven Orszag of Cambridge Hydrodynamics, Inc.

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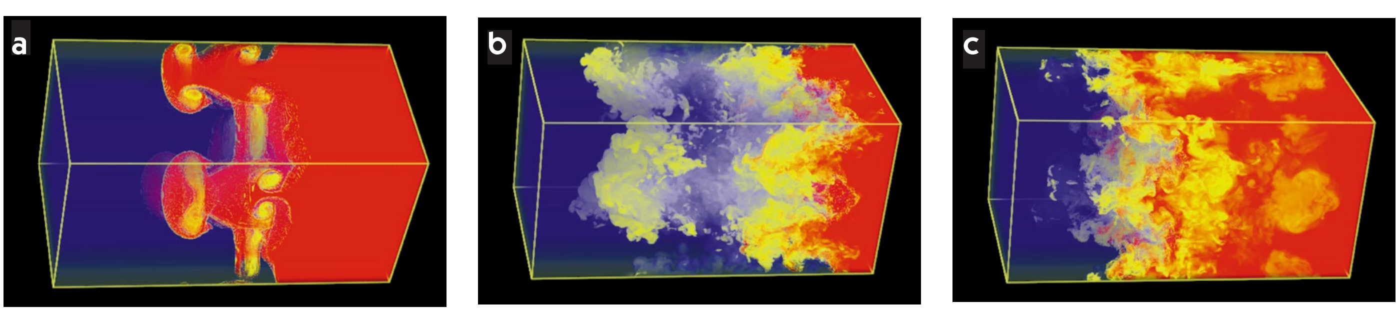

Figure 3. A passive scalar used to indicate the degree of mixing, for the Richtmyer-Meshkov problem. Blue indicates low density, and red high density.

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